One-electron model
for graphene-like materials

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Workshop on Mathematical and Physical Aspects of Topologically Protected States

Columbia University
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Collaborations

Honeycomb Schroedinger operators
C.L. Fefferman (Princeton)

J.P. Lee-Thorp (Courant - NYU)

Maxwell's eqns - Planar electromagnetic honeycomb optical media
w/ Y. Zhu (Tsinghua)

Semi-classical wavepackets and Berry curvature -
w/ J. Lu (Duke) and A. Watson (Columbia $\longrightarrow$ Duke)

Lieb Lattice,. . .
w/ R. Keller (Columbia), J. Marzuola (UNC), B. Osting (Utah)

Experimental collaborations (photonic waveguides):
N. Yu (Columbia - Applied Physics), Wong (UCLA - EE),
Z. Yu (Wisconsin - EE)

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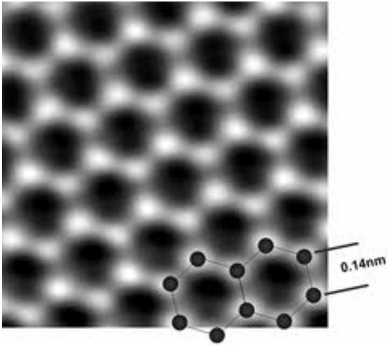
Graphene: 2- dimensional honeycomb arrangement of **C** atoms

$$i\partial_t\psi = (\ -\Delta + V(\mathbf{x})\ )\,\psi$$



A. Geim, K. Novoselov

Novel electronic properties related to “Dirac cones” of dispersion surfaces

“Artificial”, e.g. “Photonic Graphene”
Honeycomb arrays of optical waveguides

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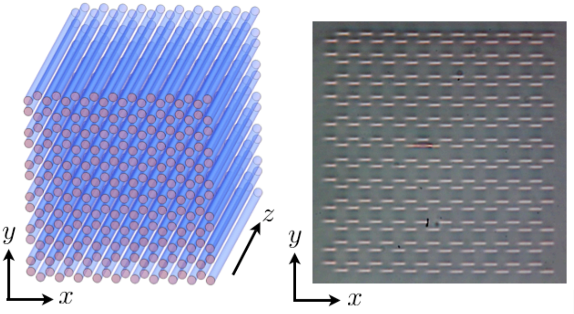
Paraxial Schroedinger equation: $i\partial_z\psi = (\ -\Delta + V(x, y)\ )\,\psi$



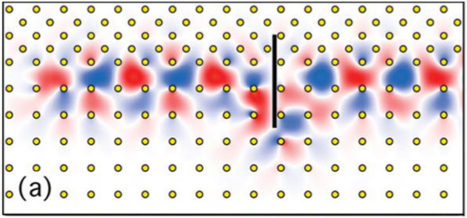
(a) (b)

Segev, Rechtsman, Szameit *et. al.*

Photonic edge states in planar structures -
Haldane-Raghu (2008), Soljacic *et al* (2008)

Maxwell's equations – TM modes

$$-\nabla_\perp \cdot \varepsilon(\mathbf{x}_\perp)\nabla H_z = \omega^2 H_z, \qquad \varepsilon(\mathbf{x}_\perp) = \begin{pmatrix} \varepsilon_0(\mathbf{x}_\perp) & -ib(\mathbf{x}_\perp) \\ ib(\mathbf{x}_\perp) & \varepsilon_0(\mathbf{x}_\perp) \end{pmatrix}$$



Several striking features:

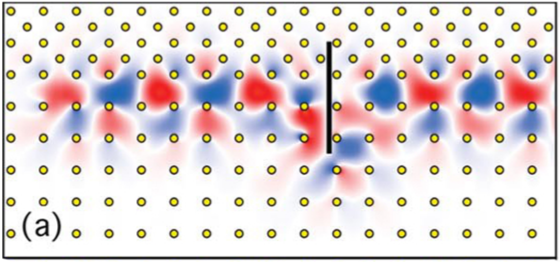
1) waves are propagating in only one direction.

2) when introducing the perturbation, localization at the interface persists.

3) when the propagating waves encounter the barrier, they do not reflect back or scatter into the "bulk". Rather the waves circumnavigate the barrier.

Why are topologically protected edge states interesting?

- The existence of these states is stable to local, even large, perturbations of the interface!
- No scattering backward and (essentially) none into the bulk!
- Mechanisms for very robust energy transfer with great potential for nanotechnologies,. . .



In condensed matter physics, such edge states are the hallmark of “topological insulators”.

The mechanisms for such transport are present and are being actively explored, both theoretically and experimentally, in condensed matter physics, acoustics, elasticity, mechanics,. . .

How such topologically protected edge states arise from the underlying continuum PDEs of Wave Physics is one of the goals of this research.

Outline

- Honeycomb structures and honeycomb lattice potentials,

$$H^\lambda = -\Delta + \lambda^2 V(\mathbf{x})$$

Example:

$$V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbb{H}} V_{\text{atomic well}}(\mathbf{x}+\mathbf{v})$$

- Dirac points - conical singularities in the band structure of H^λ

$\lambda > 0$ small (nearly free electron)

λ generic (no constraint on size)

$\lambda > \lambda_\star$ strong-binding regime and the Wallace TB-model (1947)

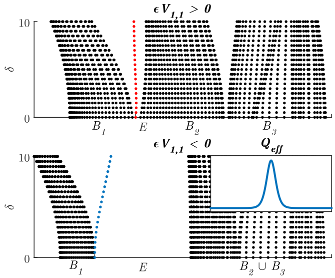
- Stability and instability of Dirac Points ($\mathcal{P}\circ\mathcal{C}$ symmetry)

- Edges – extended line-defects – in honeycomb structures

- Topologically protected edge states in honeycomb structures -

Robust bifurcation from conical intersection of continuum spectral bands

A bifurcation perspective on edge states localized on a domain wall, $\kappa(\zeta)$



Top: Bifurcation from linear (conical) crossing of bands, seeded by protected $0-$ energy eigenmode of an effective (massless) Dirac operator

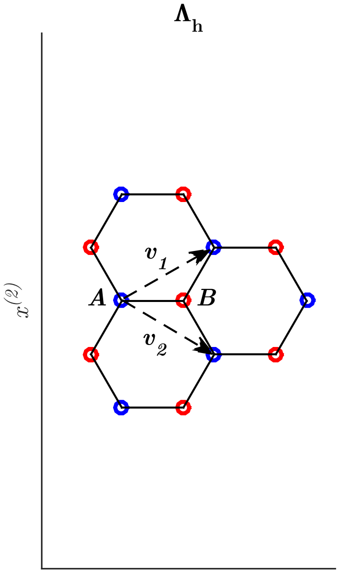
$$\mathcal{D}\alpha_\star(\zeta) \equiv \left(i\, v_F\, \sigma_3 \frac{\partial}{\partial\zeta} + \vartheta_\sharp \kappa(\zeta)\sigma_1 \right) \alpha_\star(\zeta) = 0\,, \quad v_F\, \vartheta_\sharp \neq 0$$

Bottom: (More typical) Band-edge bifurcation is seeded by point e-values of an effective massive Schroedinger operator:

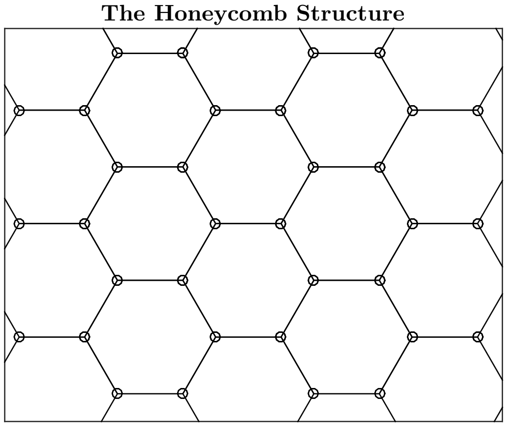
$$H_{\rm eff} \equiv -\frac{1}{2m_{\rm eff}} \frac{\partial^2}{\partial\zeta^2} + Q_{\rm eff}[\kappa](\zeta), \quad m_{\rm eff} < 0$$

Honeycomb structures and Honeycomb lattice potentials,

$$\mathbf{H} = (\mathbf{A} + \Lambda) \cup (\mathbf{B} + \Lambda)$$

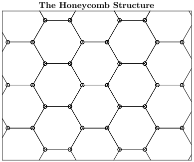


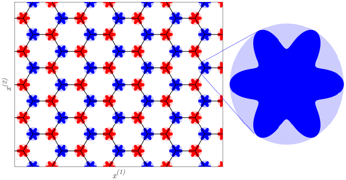
$\mathbf{H} = (\mathbf{A} + \Lambda) \cup (\mathbf{B} + \Lambda)$



Example: Let $V_0(\mathbf{x})$ be a compactly supported real-valued, radial (or appropriately symmetric) potential

$$V(\mathbf{x}) \equiv \sum_{\mathbf{w}\in\mathbf{H}} V_0(\mathbf{x}+\mathbf{w}), \qquad \mathbf{H} = (\mathbf{A}+\Lambda) \cup (\mathbf{B}+\Lambda)$$





The potential $V(\mathbf{x}) \equiv \sum_{\mathbf{w}\in\mathbf{H}} V_0(\mathbf{x}+\mathbf{w})$

is an example of a Honeycomb lattice potential.

Honeycomb lattice potentials; $H \equiv -\Delta + V(\mathbf{x})$

With respect to an appropriate origin of coordinates:

1. $V(\mathbf{x})$ is Λ_h- periodic: $V(\mathbf{x}+\mathbf{v}) = V(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^2$ and $\mathbf{v} \in \Lambda_h$.
2. $V(\mathbf{x})$ is real and inversion-symmetric: $V(-\mathbf{x}) = V(\mathbf{x})$
3. $V(\mathbf{x})$ is invariant under 120° rotation :

$$\mathcal{R}[V](\mathbf{x}) \equiv V(R^*_{120}\mathbf{x}) = V(\mathbf{x})$$

Waves in a honeycomb structure

We consider the Schroedinger equation:

$$i\partial_t\psi \;=\; (\,-\Delta + V(\mathbf{x})\,)\,\psi, \qquad V(\mathbf{x}+\mathbf{v}) = V(\mathbf{x}) \text{ for all } \mathbf{v} \in \Lambda_h,$$

where $V(\mathbf{x})$ is a honeycomb potential.

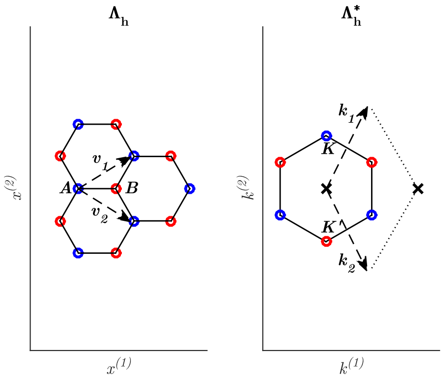
- Single electron model in QM
- Paraxial approximation in E&M
- Many of our results apply to 2D-Maxwell

Spectral theory of $H_V = -\Delta + V$ (Floquet-Bloch)

For each "quasi-momentum" $\mathbf{k} \in \mathcal{B}$, seek : $u(x;\mathbf{k}) = e^{i\mathbf{k}\cdot x} p(x;\mathbf{k})$,

$$H(\mathbf{k})\, p(\mathbf{x};\mathbf{k}) \;\equiv\; \Big(-(\nabla + i\mathbf{k})^2 + V(\mathbf{x}) \Big)\, p(\mathbf{x};\mathbf{k}) = E(\mathbf{k}) p(\mathbf{x};\mathbf{k}),$$

$$p(\mathbf{x}+\mathbf{v};\mathbf{k}) \;=\; p(\mathbf{x};\mathbf{k}), \;\; \text{all} \;\; \mathbf{v} \in \Lambda, \;\; \mathbf{x} \in \mathbb{R}^2$$



The band structure of $-\Delta + V(\mathbf{x})$.

The EVP has, for each $\mathbf{k} \in \mathcal{B}$, a discrete sequence of e-values:

$$E_1(\mathbf{k}) \leq E_2(\mathbf{k}) \leq E_3(\mathbf{k}) \leq \cdots \leq E_b(\mathbf{k}) \leq \ldots$$

with Λ periodic eigenfunctions $p_b(\mathbf{x}; \mathbf{k}),\ b = 1, 2, 3, \ldots$

The band structure of $-\Delta + V(\mathbf{x})$.

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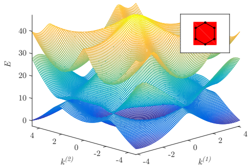
with Λ periodic eigenfunctions $p_b(\mathbf{x}; \mathbf{k})$, $b = 1, 2, 3, \ldots$

The mappings $\mathbf{k} \in \mathcal{B} \mapsto E_b(\mathbf{k})$, $b = 1, 2, 3, \ldots$
are called **dispersion relations** of $-\Delta + V$

The graphs $E_b(\mathbf{k})$ vs. $\mathbf{k} \in \mathcal{B}$ are called **dispersion surfaces**.

$$L^2(\mathbb{R}^2) - \text{ spectrum}(-\Delta + V) \ = \ E_1(\mathcal{B}) \cup E_2(\mathcal{B}) \cup E_3(\mathcal{B}) \cup \ldots E_b(\mathcal{B}) \cup \ldots$$

First 3 dispersion surfaces of $-\Delta + V_{\text{honeycomb}}(\mathbf{x}),\ E_b(\mathbf{k}),\ b = 1, 2, 3$:



A conical intersection of dispersion surfaces is often called a Dirac point.

Conical / Dirac / Diabolical / Hamilton points – a long history

3D: Spatially homogeneous ani-isotropic Maxwell equations

Symmetry: Polarization degeneracy (vector character)

Dispersion relation (polynomial): Conical singularities $\Longrightarrow$ Conical diffraction

Hamilton (1837), Ludwig (1961), Uhlmann (1982), Berry (1983, 2007), . . .

More precisely, what is a Dirac point ?

Definition A Dirac Point is a quasi-momentum / energy pair $(\mathbf{K}_\star, E_D)$, such that for $\mathbf{k}$ near $\mathbf{K}_\star$:

$$E_\pm(\mathbf{k}) - E_D \approx \pm v_F \left|\mathbf{k} - \mathbf{K}_\star\right|, \quad \text{with } v_F > 0 \text{ “Fermi velocity”}$$

Prop: Conditions ensuring existence of a Dirac point at $(\mathbf{K}_\star, E_D)$:

(P1) 2-fold degeneracy:

$$\begin{aligned} H\Phi_1 &= E_D\Phi_1, \quad \Phi_1(\mathbf{x}+\mathbf{v}) = e^{i\mathbf{K}_\star\cdot\mathbf{v}}\Phi_1(\mathbf{x}),\ \Phi_1(R^\star_{120}\mathbf{x}) = \tau\Phi_1(\mathbf{x}) \\ H\Phi_2 &= E_D\Phi_2 \quad \Phi_2(\mathbf{x}+\mathbf{v}) = e^{i\mathbf{K}_\star\cdot\mathbf{v}}\Phi_2(\mathbf{x}),\ \Phi_2(R^\star_{120}\mathbf{x}) = \bar{\tau}\Phi_2(\mathbf{x}) \end{aligned}$$

(P2) $\Phi_2(\mathbf{x}) = \overline{\Phi_1(-\mathbf{x})} = (\mathcal{P}\circ\mathcal{C})[\Phi_1]$, (aka PT symmetry)

(P3) $v_F = \left| \langle\Phi_1, \partial\Phi_2\rangle \right| > 0$

Honeycomb lattice potentials, V, and Dirac Points; Fefferman & W JAMS '12

$$H^\lambda = -\Delta + \lambda^2 V(\mathbf{x}), \qquad V_{1,1} \neq 0 \ \text{(non-degeneracy)}$$

Thm 1: (Fefferman-W. - JAMS, 2012)

Generic honeycomb potentials have Dirac points at vertices of $\mathcal{B}_h$

(a) Generic λ: For $\lambda \notin \mathbb{R} \setminus \mathcal{C}_{\text{Bad}}$ where $\mathcal{C}_{\text{Bad}}$ is discrete,
H^λ has Dirac points in its band structure

$$E^\lambda_\pm(\mathbf{k}) - E^\lambda_\star \approx \pm v^\lambda_F \, |\mathbf{k} - \mathbf{K}_\star| \,, \quad \text{with } \underline{v^\lambda_F > 0}$$

No restriction on size of λ.

(b) for all $\lambda > 0$ small and $V_{1,1} > 0$:
Dirac points occur at intersections of 1^{st} and 2^{nd} dispersion surfaces.

(c) for all $\lambda > 0$ small and $V_{1,1} < 0$:
Dirac points occur at intersections of 2^{nd} and 3^{rd} dispersion surfaces.

N.B. The set $\mathcal{C}_{\text{Bad}}$ may not be empty.

Examples with Dirac point *exchanges*, *e.g.* Bands $(2,3) \longrightarrow (1,2)$ as $\lambda \uparrow$.

Related rigorous mathematical work on Dirac points in periodic structures:

Schroedinger operators:

Colin de Verdiere (1991); Grushin (2009); Berkolaiko-Comech (2014),
Lee (point scatterers) (2016);

Quantum graph models:

Kuchment-Post (carbon nanotubes) - (2007),
Do-Kuchment (graphyne) -(2013);

Maxwell's eqns (isotropic and anisotropic):

Lee-Thorp, W. & Zhu (2016-17)

Effective 2D Dirac dynamics

Theorem (Fefferman-W. CMP - 2014)

$$i\partial_t\psi \;=\; \left(-\Delta + \lambda^2 V_h(\mathbf{x})\right)\psi, \qquad\qquad (\lambda \notin \mathcal{C}_{Bad})$$

Wave packet initial data: $\|\psi_0^\delta\|_{L^2} = \mathcal{O}(1)$ bandwidth $\delta \ll 1$ about Dirac pt :

$$\psi_0^\delta(\mathbf{x}) \;=\; \delta\;(\;\alpha_{10}(\delta\mathbf{x})\;\Phi_1(\mathbf{x}) + \alpha_{20}(\delta\mathbf{x})\;\Phi_2(\mathbf{x})\;)\;,\quad \alpha_{10},\; \alpha_{20}\quad \text{decaying at infty}$$

$$t>0 \qquad \psi^\delta(\mathbf{x},t) = e^{-i\mu_\star t}\left(\sum_{j=\pm}\delta\,\alpha_j(\delta\mathbf{x},\delta t)\Phi_j(\mathbf{x}) + \eta^\delta(\mathbf{x},t)\right)\;,$$

Dirac-type Effective eqns for $\alpha(\mathbf{X},T)$:

$$\begin{aligned}\partial_T\alpha_1 &= -\overline{z_\sharp}\;(\partial_{X_1} + i\partial_{X_2})\;\alpha_2\\ \partial_T\alpha_2 &= -z_\sharp\;(\partial_{X_1} - i\partial_{X_2})\;\alpha_1\end{aligned}$$

$z_\sharp \in \mathbb{C}$ depends on degen. Bloch modes: Φ_1 and Φ_2, and $|z_\sharp| = v_F > 0$.

Error est: $\sup_{0\le t\le\delta^{-2+100\varepsilon_1}} \left\|\,\partial_{\mathbf{x}}^\alpha\eta^\delta(\mathbf{x},t)\,\right\|_{L^2(\mathbb{R}^2_{\mathbf{x}})} \;\le\; C_{\varepsilon_1}\;\delta^{\varepsilon_1}$ as $\delta \to 0$.

Why do Dirac points appear at the vertices of the Brillouin zone $\mathcal{B}$?

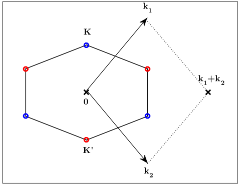
$H^\lambda = -\Delta + \lambda^2 V(\mathbf{x})$

$\lambda = 0$: $-\Delta\Psi = E^0_\star\Psi$

3$-$ dim. eigenspace: $\mathrm{span}\{e^{i\mathbf{K}\cdot\mathbf{x}},\ e^{iR\mathbf{K}\cdot\mathbf{x}},\ e^{iR^2\mathbf{K}\cdot\mathbf{x}}\}$,

degenerate e-value: $E^0_\star = |\mathbf{K}|^2 = |R\mathbf{K}|^2 = |R^2\mathbf{K}|^2$, $\quad R = 120^\circ$ rotation

The Brillouin Zone is a Fundamental Domain for $\mathbb{R}^2/\Lambda_h^*$



Extra symmetry: $[H(\mathbf{K}_\star), \mathcal{R}] = 0$, $\mathcal{R}[f](\mathbf{x}) \equiv f(R^*\mathbf{x})$ has e-values $1, \tau, \overline{\tau}$

$\lambda \neq 0$:

(a) λ small, IFT. $\quad E^0$ splits into $E^\lambda_D \in L^2_{\mathbf{K},\tau} \oplus L^2_{\mathbf{K},\overline{\tau}}$ and $\tilde{E}^\lambda \in L^2_{\mathbf{K},1}$ $(\tilde{E}^\lambda \neq E^\lambda_D)$

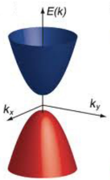
(b) Continuation in λ: $\lambda \mapsto v^\lambda_F \times \det_2(I + T^\lambda_{\mathbf{K},1}) \neq 0$

Stability / Instability of Dirac Points: $\mathcal{P}[f](\mathbf{x}) = f(-\mathbf{x})$, $\mathcal{C}[f](\mathbf{x}) = \overline{f(\mathbf{x})}$

Thm 2: (Stability)
Dirac points persist against small perturbations of $-\Delta + V_h$, which preserve $\mathcal{P} \circ \mathcal{C}$, *i.e.* one may break rotational invariance.

(...but "Dirac cones" may perturb away from the vertices of $\mathcal{B}_h$)

Thm 3: (Instability)
If $\mathcal{P}$ or $\mathcal{C}$ is broken then the dispersion surfaces are smooth in a neighborhood of the vertices of $\mathcal{B}_h$.



N.B. However, spectral gap may open <u>only locally</u> in **k** !

Dispersion surfaces may <u>"fold over"</u> away from the vertices of $\mathcal{B}_h$.

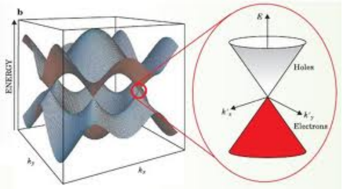
Tuning of the physics

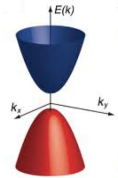
- $\mathcal{C}-$ or $\mathcal{P}-$ breaking deformations cause the material to

  transition between “phases”:

  (i) conduction (no gap) $\rightleftharpoons$ insulation (gapped)

  (ii) non-dispersive waves (Dirac) $\rightleftharpoons$ dispersive waves (Schrödinger)



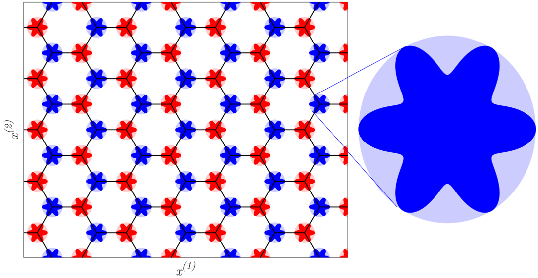


- We will take advantage of this instability of Dirac points (to symmetry breaking perturbations) to construct “protected edge states” with energies in a spectral gap.

Dirac points in the strong binding regime

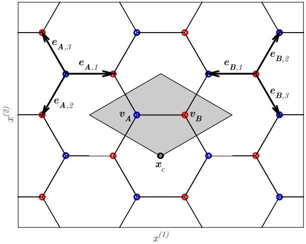
We study the continuous Schroedinger operator $-\Delta + \lambda^2 V(\mathbf{x})$, with *honeycomb lattice potential* $V(\mathbf{x})$ defined on $\mathbb{R}^2$ and $\lambda > \lambda_\star$ sufficiently large.

$V(\mathbf{x}) \; = \; \sum_{\mathbf{v} \in \mathbf{H}} \; V_0(\mathbf{x})$ superposition of "atomic potential wells":



Hypotheses on atomic potential, $V_0(\mathbf{x})$ $\left[V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x}+\mathbf{v})\right]$

1. V_0 is a potential well with support in $B_{r_0}(0)$, with $0 < r_0 \lesssim .33\ a_{lattice}$
2. $V_0(-\mathbf{x}) = V_0(\mathbf{x}),\ \ V_0(R^*_{120}\mathbf{x}) = V_0(\mathbf{x})$
3. $(p_0^\lambda, E_0^\lambda)$, ground state of $-\Delta + \lambda^2 V_0$: $E_0^\lambda \leq -C\lambda^2$
4. $\langle(-\Delta + \lambda^2 V_0 - E_0^\lambda)\psi, \psi\rangle \geq c_{gap}\, \|\psi\|^2$, all $\psi \perp p_0^\lambda$ $\quad$ (c_{gap} indep. of λ)



Floquet-Bloch spectrum of $H^\lambda = -\Delta + \lambda^2 V(\mathbf{x}), \ V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x})$

k- dependent Hamiltonian: $H^\lambda(\mathbf{k}) = -(\nabla + i\mathbf{k})^2 + \lambda^2 V(\mathbf{x}), \ \mathbf{k} \in \mathcal{B}_h$

Λ_h- periodic eigenvalues of $H^\lambda(\mathbf{k})$: $E_1^\lambda(\mathbf{k}) \leq E_2^\lambda(\mathbf{x}) \leq \cdots \leq E_b^\lambda(\mathbf{k}) \leq \cdots$

Dispersion surfaces: $\mathbf{k} \in \mathcal{B}_h \mapsto E_b^\lambda(\mathbf{k})$, b=1,2,3,...

Problem: For λ sufficiently large, describe the low-lying dispersion surfaces of H^λ, obtained from 2 lowest eigenvalues of $H^\lambda(\mathbf{k})$:

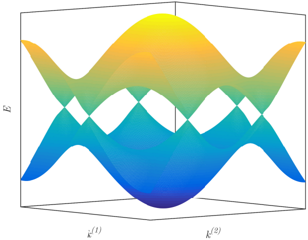
$$\mathbf{k} \mapsto E_1^\lambda(\mathbf{k}) = E_-^\lambda(\mathbf{k}) \quad \text{and} \quad \mathbf{k} \mapsto E_2^\lambda(\mathbf{k}) = E_+^\lambda(\mathbf{k}),$$

$$H^{\lambda} = -\Delta + \lambda^2 V(\mathbf{x}), \qquad V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x})$$

For all $\lambda > \lambda_\star$ sufficiently large, the two lowest dispersion surfaces,

$$\mathbf{k} \in \mathcal{B}_h \mapsto E^{\lambda}_{\pm}(\mathbf{k}),$$

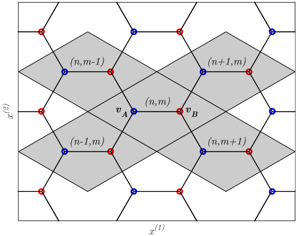
upon a (V_0- dependent) rescaling, converges to a universal limit.



The 2-band tight-binding model of PR Wallace[1]

[1] *The band structure of graphite, Phys. Rev. (1947)*

Two band tight-binding model- *P.R. Wallace, 1947*



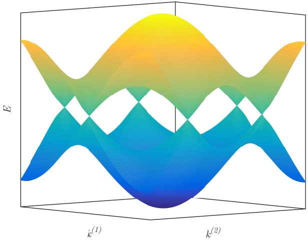
$$i\partial_T\ \psi_A^{n,m} = t\left[\ \psi_B^{n,m} + \psi_B^{n,m-1} + \psi_B^{n-1,m}\ \right]$$

$$i\partial_T\ \psi_B^{n,m} = t\left[\ \psi_A^{n,m} + \psi_A^{n+1,m} + \psi_A^{n,m+1}\ \right]$$

Dispersion relation: $\begin{pmatrix}\psi_A^{n,m}\\ \psi_B^{n,m}\end{pmatrix} = e^{i(\mathbf{k}\cdot(n\mathbf{v}_1+m\mathbf{v}_2)\ -\Omega\ T)}\begin{pmatrix}\xi_A\\ \xi_B\end{pmatrix},\ \mathbf{k}\in\mathcal{B}$

$$\Omega_\pm(\mathbf{k}) = \pm\, t\,\mathcal{W}_{TB}(\mathbf{k}),\quad \mathcal{W}_{TB}(\mathbf{k}) = \left|1 + e^{i\mathbf{k}\cdot\mathbf{v}_1} + e^{i\mathbf{k}\cdot\mathbf{v}_2}\right|$$

Dirac Points in the Band structure of Wallace's 2-band tight-binding model



$$\Omega_{\pm}(\mathbf{k}) \;=\; \pm\, t\, \mathcal{W}_{TB}(\mathbf{k}), \quad \mathcal{W}_{TB}(\mathbf{k}) = \left| 1 + e^{i\mathbf{k}\cdot\mathbf{v}_1} + e^{i\mathbf{k}\cdot\mathbf{v}_2} \right|$$

<u>Conical singularities</u> - Dirac points

Precise statement of Th'm on the Strong Binding Regime:

- **Scaling limit:** there exists an energy $E_D^\lambda \approx E_0^\lambda$ such that

  for any vertex $\mathbf{K}_\star$ of $\mathcal{B}_h$, the pair $(E_D^\lambda, \mathbf{K}_\star)$ is a Dirac point

- there exists $\rho_\lambda > 0$ such that as $\lambda \to \infty$:

  $$\left(E_-^\lambda(\mathbf{k}) - E_D^\lambda \right) / \rho_\lambda \to -\mathcal{W}_{TB}(\mathbf{k}) \text{ and } \left(E_+^\lambda(\mathbf{k}) - E_D^\lambda \right) / \rho_\lambda \to +\mathcal{W}_{TB}(\mathbf{k}) ,$$

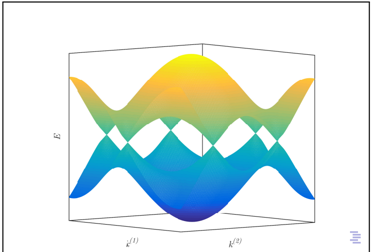
  uniformly in $\mathbf{k} \in \mathcal{B}_h$.

  $$\mathcal{W}_{TB}(\mathbf{k}) \equiv \left| 1 + e^{i\mathbf{k}\cdot\mathbf{v}_1} + e^{i\mathbf{k}\cdot\mathbf{v}_2} \right|, \quad \rho_\lambda \approx e^{-c\lambda} \text{ (hopping coefficient)} .$$

- For $\mathbf{K}_\star$, any vertex of $\mathcal{B}_h$:

$$\mathcal{W}_{TB}(\mathbf{k}) = \frac{\sqrt{3}}{2} |\mathbf{k} - \mathbf{K}_\star| + \mathcal{O}(|\boldsymbol{\kappa}|^2)$$

- $v_F^\lambda = \rho_\lambda \left[\frac{\sqrt{3}}{2} + \mathcal{O}(e^{-c\lambda}) \right]$



Corollary A:

Spectral gaps for $\mathcal{P} \circ \mathcal{C}$ breaking perturbations of $-\Delta + \lambda^2 V(\mathbf{x})$.

$$H^{\lambda,\eta} = -\Delta + \lambda^2 V(\mathbf{x}) + \eta W(\mathbf{x})$$

Corollary B:

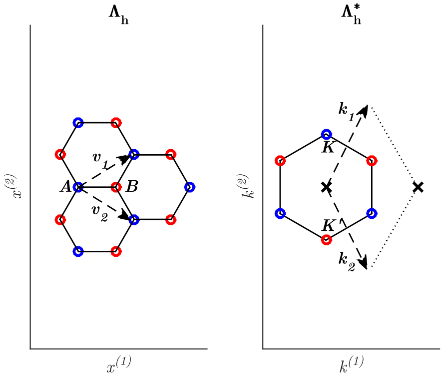
Topologically protected edge states
concentrated along rational edges (line-defects)

$$H^{(\lambda,\delta)} \equiv -\Delta + \lambda^2 V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x})W(\mathbf{x}).$$

Edge States in Honeycomb Structures

Fefferman, Lee-Thorp, W, Annals of PDE - 2016

Recall

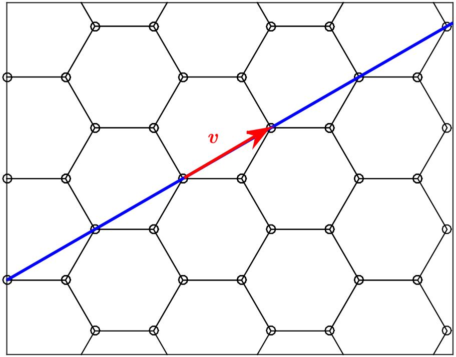


$\mathbf{k}_m \cdot \mathbf{v}_n = 2\pi\delta_{mn},$ $\mathcal{B}$

The Zigzag Edge

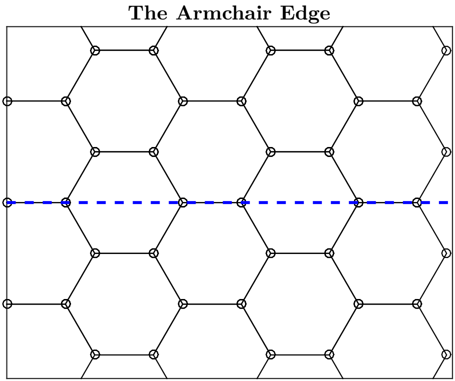
- $\mathfrak{v}_1 = \mathbf{v}_1, \mathfrak{v}_2 = \mathbf{v}_2, \ \mathfrak{K}_1 = \mathbf{k}_1$ and $\mathfrak{K}_2 = \mathbf{k}_2 \ ; \ \mathfrak{K}_m \cdot \mathfrak{v}_n = 2\pi\delta_{mn}$

The Zigzag Edge



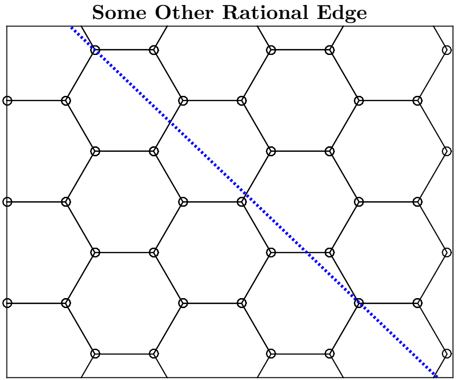
The Armchair Edge

- $\mathfrak{v}_1 = \mathbf{v}_1 + \mathbf{v}_2$, $\mathfrak{v}_2 = \mathbf{v}_2$, $\mathfrak{K}_1 = \mathbf{k}_1$, $\mathfrak{K}_2 = \mathbf{k}_2 - \mathbf{k}_1$; $\mathfrak{K}_m \cdot \mathfrak{v}_n = 2\pi\delta_{mn}$



General rational edge

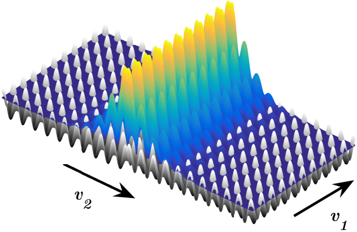
- $$\mathfrak{v}_1 = a_1\mathbf{v}_1 + b_1\mathbf{v}_2, \quad a_1, b_1 \in \mathbb{Z}, \quad (a_1, b_1) = 1, \quad \mathfrak{v}_2, \ \mathfrak{K}_1, \ \mathfrak{K}_2$$
  $$\mathfrak{K}_m \cdot \mathfrak{v}_n = 2\pi\delta_{mn}, \quad m, n = 1, 2$$



$\mathfrak{v}_1 = -\mathbf{v}_1 + 4\mathbf{v}_2$

Edge states are solutions $\psi(\mathbf{x}, t) = e^{-iEt}\Psi(\mathbf{x})$ of a wave equation (Schroedinger, Maxwell, . . .) which are

- propagating (plane-wave like) parallel to a line-defect ("edge")
- localized transverse to the edge.



- **Dirac pts provide a mechanism for producing <u>protected</u> edge states**

Models in which we construct protected edge states

- quantum and electromagentic

Motivation:

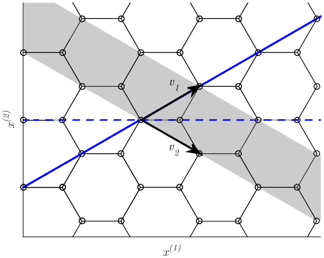
Haldane-Raghu PRL ‘08, Raghu-Haldane Phys Rev A, ‘08
Photonic realization of quantum-Hall type one-way edge states

Wang, Chong, Joannopoulos & Soljacic PRL ‘08
Reflection free one-way edge modes in a gyromagnetic photonic crystal

See also M. Rechtsman *et. al.*, A. Khanikaev *et. al.*

Su-Schrieffer-Heeger PRL ‘79
Soliton in polyacetelene

Domain-wall-interpolation between 2 perturbed honeycombs across a line-defect



- Schroedinger – $-\Delta + V$
- Quantum dimer arrays w/ domain-wall induced phase shift, Fefferman, Lee-Thorp, W. : PNAS, '14, Memoirs AMS - 2017
- E&M / 2D Maxwell: $H^\delta = -\nabla_\perp \cdot [\epsilon_h(\mathbf{x}_\perp) + \delta\mathcal{A}(\mathbf{x}_\perp, \delta\mathfrak{K}_2 \cdot \mathbf{x}_\perp)]\, \nabla_\perp$ w/ J.P. Lee-Thorp and Y. Zhu (in prep.)

Domain-wall-interpolation between 2 perturbed honeycombs across a line-defect

Domain wall function:
$\kappa(0) = 0$ and $\kappa(\zeta) \to \pm\kappa_\infty$ as $\zeta \to \infty$

$$\underline{\text{Schroedinger:}} \qquad H^\delta \; = \; -\Delta + V_h(\mathbf{x}) \; + \; \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x}) \; W(\mathbf{x})$$

a) $V_h(\mathbf{x})$ is a honeycomb potential ($\implies$ Dirac points)

b) W is Λ_h periodic and $W(-\mathbf{x}) = -W(\mathbf{x})$ (breaks inversion symmetry)

- $\mathfrak{K}_2 \cdot \mathbf{x} \to -\infty \quad \implies \quad H^\delta \to H^\delta_\pm = -\Delta + V(\mathbf{x}) \; - \; \delta\kappa_\infty \; W(\mathbf{x})$
- $\mathfrak{K}_2 \cdot \mathbf{x} \to +\infty \quad \implies \quad H^\delta \to H^\delta_\pm = -\Delta + V(\mathbf{x}) \; + \; \delta\kappa_\infty \; W(\mathbf{x})$

$$H^\delta = -\Delta + V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x})\, W(\mathbf{x})$$

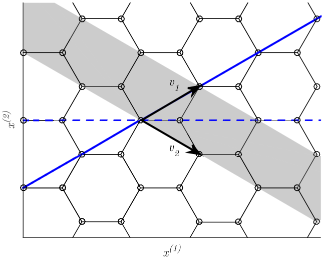
H^δ has a translation invariance, $\mathbf{x} \to \mathbf{x} + \mathfrak{v}_1$

and an associated *parallel quasi-momentum*, $k_\parallel$

The $\mathfrak{v}_1-$ edge state eigenvalue problem

$$H^\delta \Psi = E\,\Psi, \quad \Psi(\mathbf{x} + \mathfrak{v}_1) = e^{ik_\parallel}\Psi(\mathbf{x}), \quad \Psi(\mathbf{x}) \to 0, \ |\mathbf{x}\cdot\mathfrak{K}_2| \to \infty$$

Equivalently, $H^\delta\Psi = E\Psi$, $\Psi \in L^2_{k_\parallel}(\Sigma)$, $\Sigma = \mathbb{R}^2/\mathbb{Z}\mathfrak{v}_1$.



General conditions for existence of edge states, spectrally localized near Dirac pt

Thm 5: $H^\delta \; = -\Delta + V(\mathbf{x}) \; + \; \delta\kappa(\delta\, \mathfrak{K}_2 \cdot \mathbf{x})\; W(\mathbf{x})$.

- Fix a rational edge, $\mathbb{R}\mathfrak{v}_1$
- Assume $-\Delta + V$ satisfies <u>spectral no-fold condition</u> (for $\mathbb{R}\mathfrak{v}_1$)

1. There exist solutions to the edge state EVP:

$$H^\delta \Psi = E\Psi, \quad \Psi \in L^2_{k_\parallel}(\Sigma)$$

   which are spectrally supported near Dirac points of the bulk structure.

   Specifically, the EVP has a branch of eigenpairs $\delta \mapsto (\Psi^\delta, E^\delta)$ which bifurcates from the Dirac point:

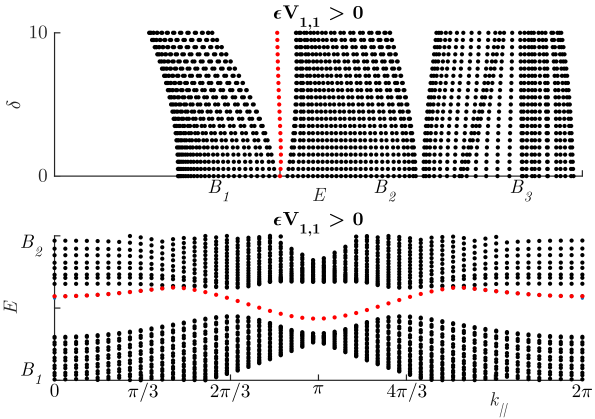
$$\Psi^\delta(\mathbf{x}) \; \approx_{H^2_{k_\parallel}} \; \alpha_{\star,+}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_-(\mathbf{x})$$

$$E^\delta = E_\star \; + \; \mathcal{O}(\delta^2).$$

2. $\alpha_\star(\zeta)$ is a 0-energy eigenstate, $\mathcal{D}\alpha_\star = 0, \; \alpha_\star \in L^2(\mathbb{R}_\zeta)$, of the Dirac operator

$$\mathcal{D} \equiv i\, z_\sharp\, \sigma_3 \frac{\partial}{\partial \zeta} \; + \; \vartheta_\sharp \underbrace{\kappa(\zeta)}_{\text{domain wall}} \; \sigma_1$$

Edge state bifurcation from a Dirac point - E vs. δ ($k_{\|}$ fixed) and E vs. $k_{\|}$ (δ fixed)



Bifurcation of transverse-localized states from the continuous spectrum of states which are spatially extended.

Robustness of the bifurcation against a class of large perturbations:

The bifurcation of Thm 5 is seeded by

"protected" (rigid) zero mode of a Dirac operator, $\mathcal{D}$

$$\Psi^{\delta}(\mathbf{x}) \approx_{H^2_{k_\parallel}} \alpha_{\star,+}(\delta\mathfrak{K}_2\cdot\mathbf{x})\Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta\mathfrak{K}_2\cdot\mathbf{x})\Phi_-(\mathbf{x})$$

$$\mathcal{D}\alpha_\star(\zeta) \equiv \left(iz_\sharp\sigma_3\frac{\partial}{\partial\zeta} + \vartheta_\sharp\kappa(\zeta)\sigma_1 \right)\alpha_\star(\zeta) = 0\ , \quad z_\sharp\vartheta_\sharp \neq 0$$

For arbitrary domain walls ($\kappa(\zeta)\to\pm\kappa_\infty$) $\mathcal{D}$ has a zero-eigenvalue.

In particular, the branch of edge states persists

even when $\kappa(\zeta)$ is perturbed by a large (but localized) perturbation.

Remarks on the spectral no-fold hypothesis

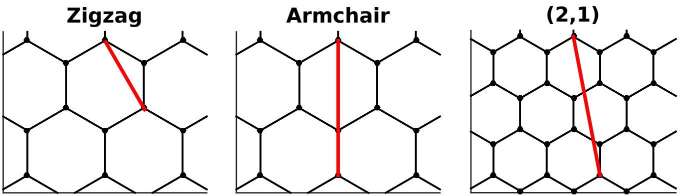
$$H^{\delta}\Psi = E\Psi, \quad \Psi \in L^2_{k_{\parallel}}(\Sigma)$$

$$\Psi(\mathbf{x}) \;=\; \sum_{b\geq 1} \int_0^1 \widetilde{\Psi}_b(\lambda)\Phi_b(\mathbf{x};\mathbf{K}+\lambda\mathfrak{K}_2)d\lambda \qquad (1)$$

$k_{\parallel}-$ pseudo-periodic in parallel to $\mathfrak{v}_1-$ and decaying as $|\mathfrak{K}_2 \cdot \mathbf{x}| \to \infty$.

(1) is continuum superposition of all Bloch modes, which are consistent with $k_{\parallel}-$ pseudo-periodicity:

$$H\,\Phi_b(\mathbf{x};\mathbf{K}+\lambda\mathfrak{K}_2) \;=\; E_b(\mathbf{K}+\lambda\mathfrak{K}_2)\,\Phi_b(\mathbf{x};\mathbf{K}+\lambda\mathfrak{K}_2)$$



Decompose into Bloch amplitudes

w/ quasi-momentum near-to and far-from the Dirac point: $\widetilde{\Psi}^{\delta}_{\pm}(\tau)$ and $\widetilde{\Psi}^{\delta}_{\rm far}(\tau)$

Bloch amplitudes $\widetilde{\Psi}^{\delta}_{\pm}(\tau)$ for quasi-momenta **near the Dirac point**

$$\left(E_-(\mathbf{K}+\tau\mathfrak{K}_2) - E_D \right) \widetilde{\Psi}_-(\tau) + \delta C^{\delta}_-[\widetilde{\Psi}_\pm(\tau), \widetilde{\Psi}_{\rm far}(\tau)] = 0$$
$$\left(E_+(\mathbf{K}+\tau\mathfrak{K}_2) - E_D \right) \widetilde{\Psi}_+(\tau) + \delta C^{\delta}_+[\widetilde{\Psi}_\pm(\tau), \widetilde{\Psi}_{\rm far}(\tau)] = 0$$

Bloch amplitudes $\widetilde{\Psi}^{\delta}_{\rm far}(\tau) = \{\widetilde{\Psi}^{\delta}_b(\tau)\}$ for quasi-momenta
far from the Dirac point

$$\left(E_b(\mathbf{K}+\tau\mathfrak{K}_2) - E_D \right) \widetilde{\Psi}_b(\tau) + \delta C^{\delta}_b[\widetilde{\Psi}_\pm(\tau), \widetilde{\Psi}_{\rm far}(\tau)] = 0$$
$$\left\{ b \neq \pm \ , \ |\tau| \le \frac{1}{2} \right\} \quad \text{or} \quad \left\{ b = \pm \ , \ \delta^{\nu} \le |\tau| \le \frac{1}{2} \right\}$$

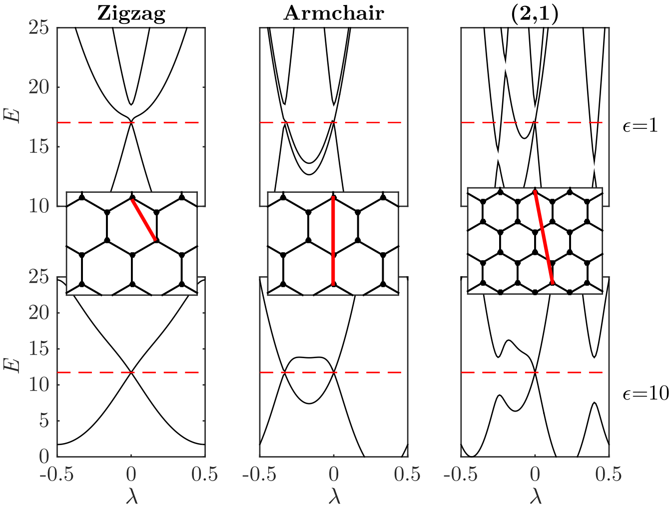
LS- reduction step: construct the map $\widetilde{\Psi}_\pm(\tau) \mapsto \widetilde{\Psi}_{\rm far}(\tau; \widetilde{\Psi}_\pm)$
to obtain closed system for $\widetilde{\Psi}_\pm(\tau)$.

Require lower bound on <u>denominators</u>:
$|E_\pm(\mathbf{K}+\tau\mathfrak{K}_2) - E^{\lambda}_D| \ge c\, \delta^{\nu}$ for all $\delta^{\nu} \le |\tau| \le 1/2$ (no-fold condition)

Study the $\mathfrak{K}_2-$slice of the band structure consisting of the union of the graphs of:

$\tau \mapsto E_b(\mathbf{K}+\tau\mathfrak{K}_2), \ \ |\tau| \le 1/2, \ \ b \ge 1, \ \ \mathfrak{K}_2 \cdot \mathfrak{v}_1 = 0, \ (\mathfrak{v}_1 = \text{edge direction})$

Band structure slices of $-\Delta + \epsilon V_h$: from low to high contrast $\to$ TB



Cases in which *spectral no-fold condition* can be proved.

Thm′s 6, 7: Existence of protected edge states (Schroedinger case)

1. Low contrast honeycomb structures –

   Protected edge states along ZIGZAG edges,
   (but not, e.g., Armchair edges)

   Proof: requires control of dispersion surfaces of $-\Delta + \lambda^2 V(\mathbf{x})$ *for* $V_{1,1} > 0$ *and* $\lambda > 0$ *small*
   – nearly free-electron Hamiltonian

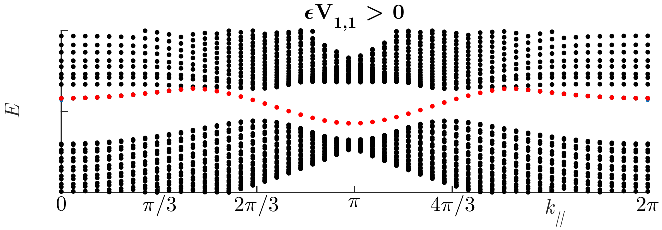
2. High-contrast honeycomb structures (deep wells / strong binding) –

   Protected edge states along "ANY" rational edge,
   i.e. $\mathfrak{v}_{a_1,a_2} = a_1\mathbf{v}_1 + a_2\mathbf{v}_2$, a_1, a_2 relatively prime integers

   Given, $\mathfrak{v}_{a_1,a_2}$, there exists $\lambda_\star(\mathfrak{v}_{a_1,a_2})$, such that for all $\lambda > \lambda_\star$ there exist protected edge states.
   Proof: Key ingredient - uniform control of dispersion surfaces in the strong binding regime

$H^\delta = -\Delta + \lambda^2 V + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x}) W(\mathbf{x})$, edge-state bifurcations for $\lambda^2 V_{1,1} > 0$

and wave-transport localized along the zigzag edge

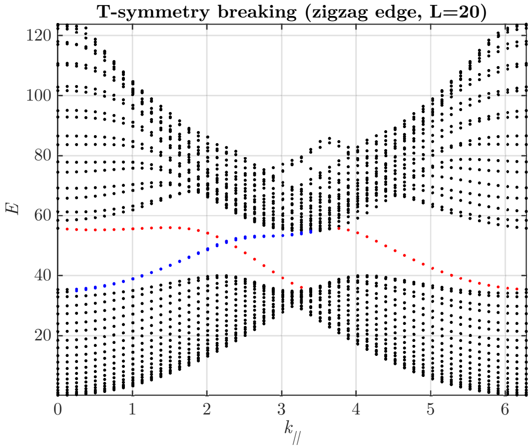


Superposition of edge states $\Longrightarrow$
wave-pkts which remain localized on the zig-zag edge and disperse along it

$$\text{left-going wave packet} \ = \int_{|k_\parallel - 2\pi/3| \ll 1} e^{i(\mathbf{K}\cdot\mathbf{x} - E(k_\parallel)t)} \ \psi(\mathbf{x}; k_\parallel) \ dk_\parallel$$

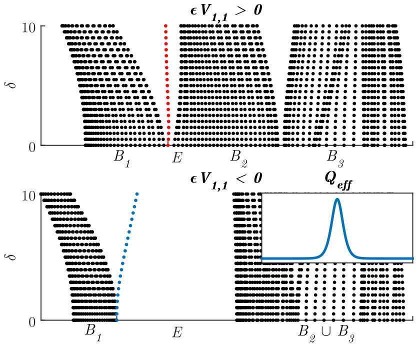
Electromagnetic (chiral) edge states in $\mathcal{C}-$ breaking media

$$H^\delta = -\nabla_\perp \cdot [\epsilon_h(\mathbf{x}_\perp) + \delta\mathcal{A}(\mathbf{x}_\perp, \delta\mathfrak{K}_2 \cdot \mathbf{x}_\perp)]\nabla_\perp$$



w/ J.P. Lee-Thorp and Y. Zhu (in preparation)

Protected (Dirac / Shockley) v. Unprotected (Schroedinger / Tamm) edge states



Dirac point bifurcation is seeded by 0$-$ energy eigenmode of Dirac op, $\mathcal{D}_{\rm eff}$

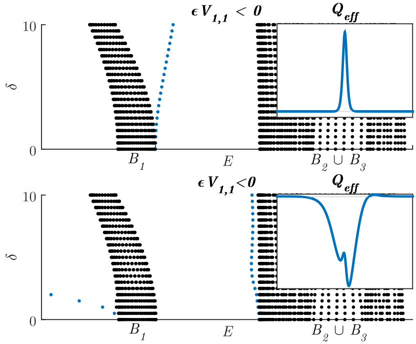
(More typical) Band-edge bifurcation is seeded by point e-values of $H_{\rm eff}$:

$$H_{\rm eff} \equiv -\frac{1}{2m_{\rm eff}} \frac{\partial^2}{\partial \zeta^2} + Q_{\rm eff}(\zeta;\kappa), \quad m_{\rm eff} < 0$$

$$Q_{\rm eff}(\zeta;\kappa) \equiv a\,\kappa'(\zeta) + b\left(\kappa_\infty^2 - \kappa^2(\zeta)\right).$$

Band-edge (Schroedinger) bifurcation can be destroyed by localized perturbation

$\kappa \to \kappa_\natural = \kappa + \text{localized}(x)$



$$H_{\text{eff}} \equiv -\frac{1}{2m_{\text{eff}}}\frac{\partial^2}{\partial\zeta^2} + Q_{\text{eff}}(\zeta;\kappa_\natural), \quad m_{\text{eff}} < 0$$

$$Q_{\text{eff}}(\zeta;\kappa) \equiv a\,\kappa_\natural'(\zeta) + b\left(\kappa_\infty^2 - \kappa_\natural^2(\zeta)\right).$$

Ongoing work and conjectures

- Notions from topology (Zak/Berry phase, Chern index,. . .),

  have played a central role in the physicists'

  classification and counting of protected edge states.

  Understood / justified only in certain tight-binding models.

  We are working on extending these arguments to the underlying PDEs.

- Topological ideas have the potential to give information on the global behavior of bifurcation curves of PDEs.

- Dynamics of semi-classical wave-packets in systems with band-degeneracies and the effect of Berry curvature
  – ongoing work with J. Lu and A. Watson

What if spectral no-fold hypothesis fails for the $\mathfrak{v}_1$ edge?

Conjecture: (based on formal asymptotic analysis and numerical evidence):

There exist meta-stable states:
long-lived states, whose energy is concentrated on the $\mathfrak{v}_1$ edge
for a very long time, but which eventually radiate their energy into the bulk.

A mathematical theory of such *protected edge "quasi-modes"*

is an interesting open challenge.

Open problem:
Irrational edges - Do irrational edge states exist?

Relation to deep mathematical problems for waves
in quasi-periodic and random media.

Thank you!